Full wwPDB NMR Structure Validation Report (i)

Feb 8, 2022 – 06:29 PM EST

PDB ID	:	1CMZ
Title	:	SOLUTION STRUCTURE OF GAIP (GALPHA INTERACTING PROTEIN): A REGULATOR OF G PROTEIN SIGNALING
Authors	:	De Alba, E.; De Vries, L.; Farquhar, M.G.; Tjandra, N.
Deposited on	:	1999-05-12

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

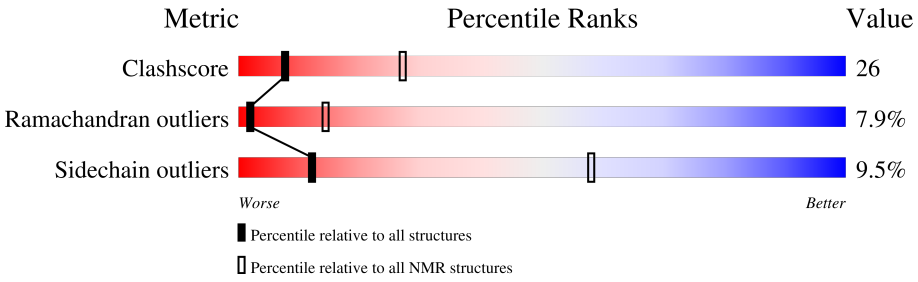
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	152	46% 29% • 5% 16%

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:79-A:148, A:156-A:206 (121)	0.36	11

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 5 single-model clusters were found.

Cluster number	Models
1	4, 5, 6, 9, 11, 12, 15, 19, 20
2	7, 16
3	1, 2
4	13, 14
Single-model clusters	3; 8; 10; 17; 18

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2069 atoms, of which 1017 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	128	2069	666	1017	180	201	5	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SER	GLN	SEE REMARK 999	UNP P49795
A	69	PRO	PRO	SEE REMARK 999	UNP P49795
A	70	GLY	LEU	SEE REMARK 999	UNP P49795
A	71	ILE	PRO	SEE REMARK 999	UNP P49795
A	72	SER	SER	SEE REMARK 999	UNP P49795
A	73	GLY	CYS	SEE REMARK 999	UNP P49795
A	74	GLY	GLU	SEE REMARK 999	UNP P49795
A	75	GLY	VAL	SEE REMARK 999	UNP P49795
A	76	GLY	CYS	SEE REMARK 999	UNP P49795
A	77	GLY	ALA	SEE REMARK 999	UNP P49795
A	78	ILE	THR	SEE REMARK 999	UNP P49795
A	207	PRO	LEU	SEE REMARK 999	UNP P49795
A	208	TRP	GLN	SEE REMARK 999	UNP P49795
A	209	VAL	GLY	SEE REMARK 999	UNP P49795
A	210	ASP	PRO	SEE REMARK 999	UNP P49795
A	212	SER	GLN	SEE REMARK 999	UNP P49795
A	215	LEU	SER	SEE REMARK 999	UNP P49795
A	216	ILE	GLU	SEE REMARK 999	UNP P49795
A	217	HIS	ALA	SEE REMARK 999	UNP P49795
A	218	ARG	-	SEE REMARK 999	UNP P49795
A	219	ASP	-	SEE REMARK 999	UNP P49795

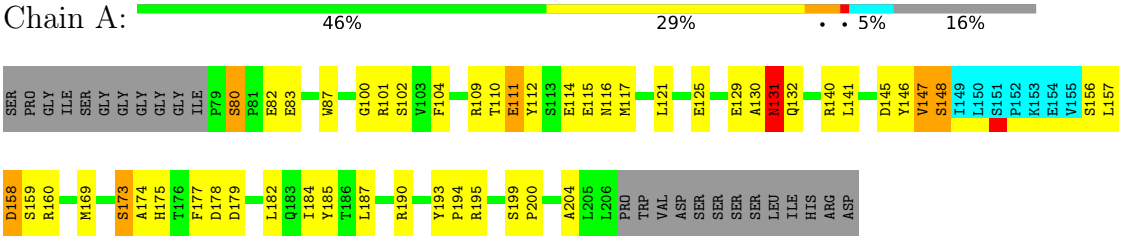
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)

Chain A:



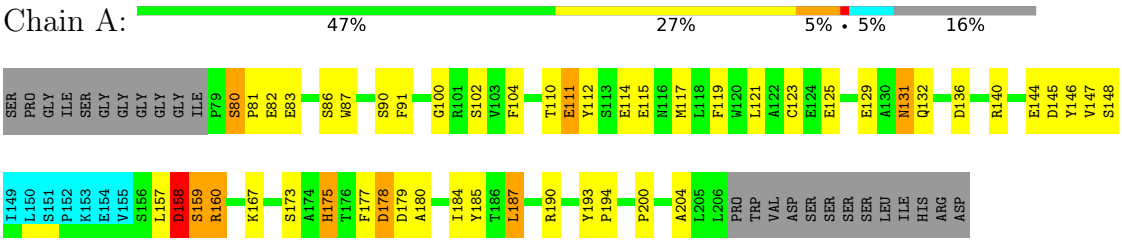
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)

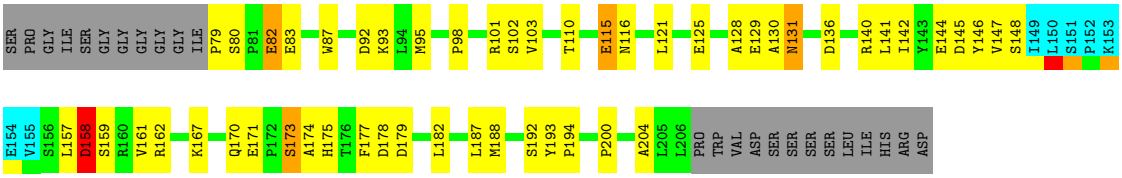
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)

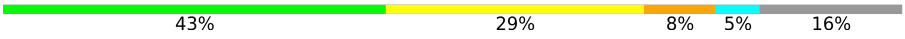
Chain A:

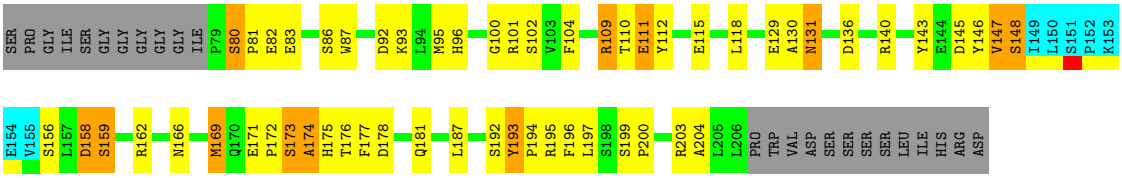


4.2.3 Score per residue for model 3

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)

Chain A:

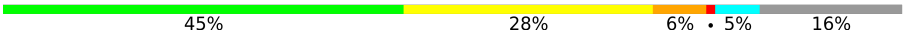


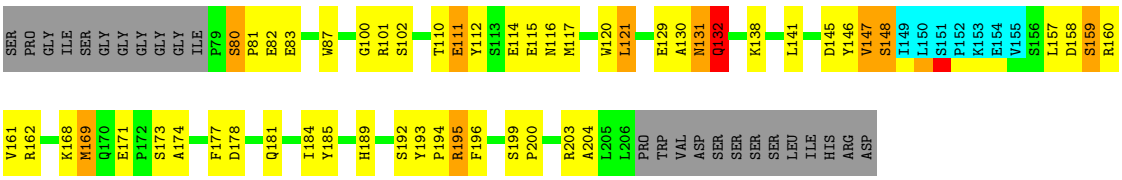


4.2.4 Score per residue for model 4

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)

Chain A:

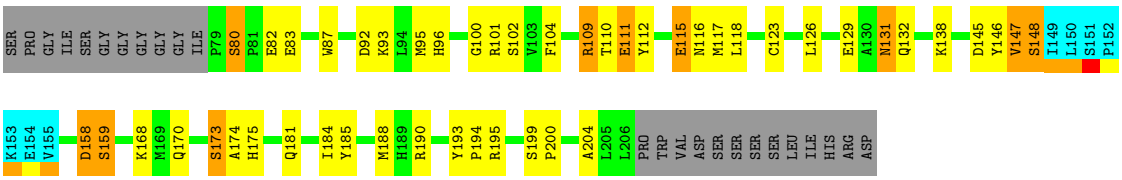




4.2.5 Score per residue for model 5

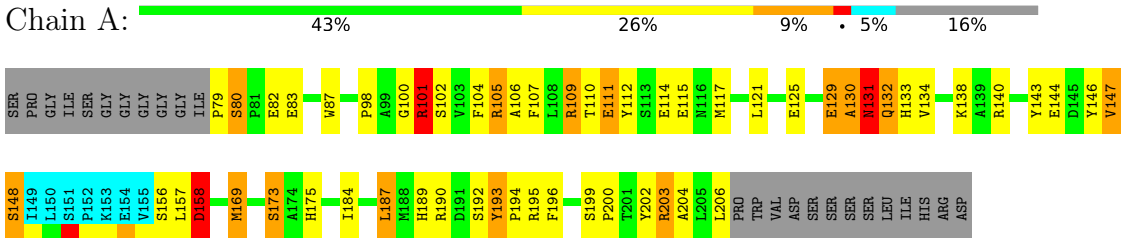
• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)

Chain A:



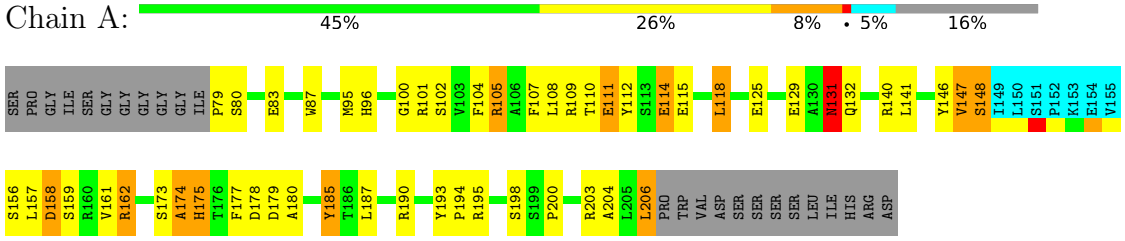
4.2.6 Score per residue for model 6

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



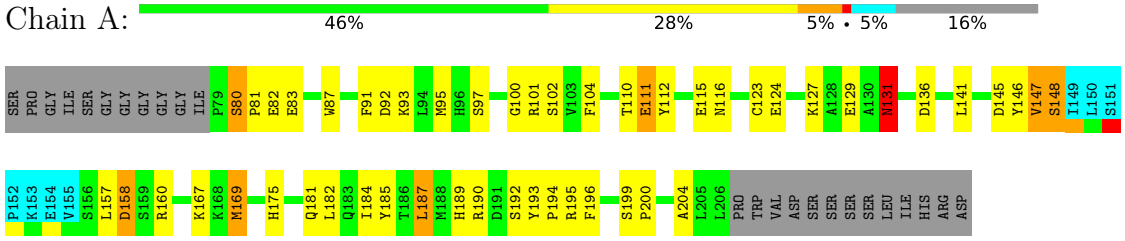
4.2.7 Score per residue for model 7

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



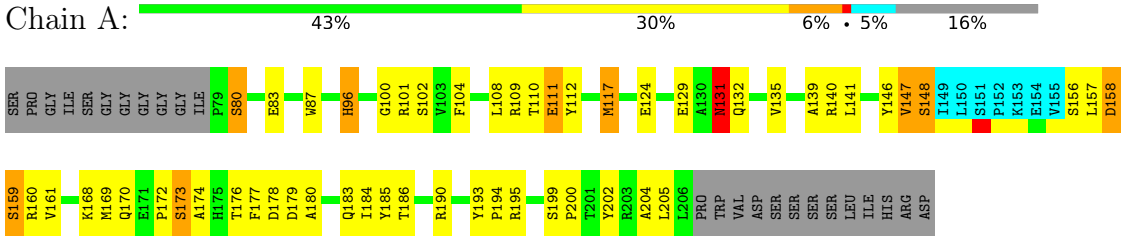
4.2.8 Score per residue for model 8

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



4.2.9 Score per residue for model 9

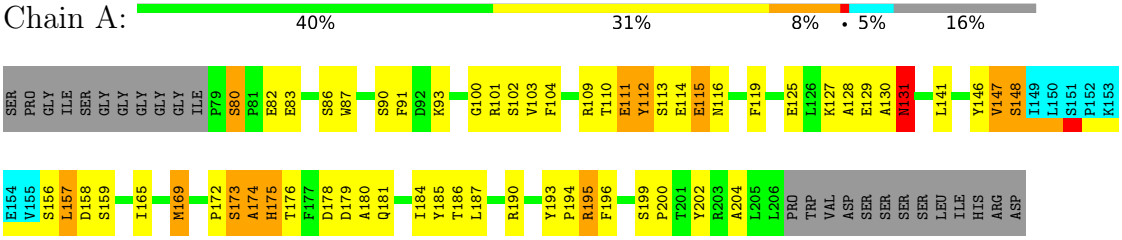
• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



4.2.10 Score per residue for model 10

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)

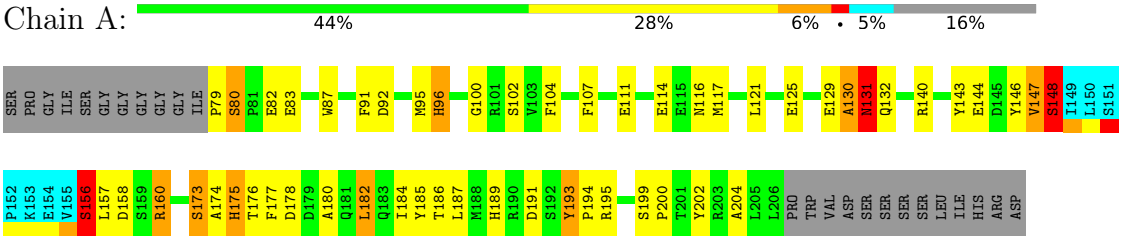
Chain A:



4.2.11 Score per residue for model 11 (medoid)

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)

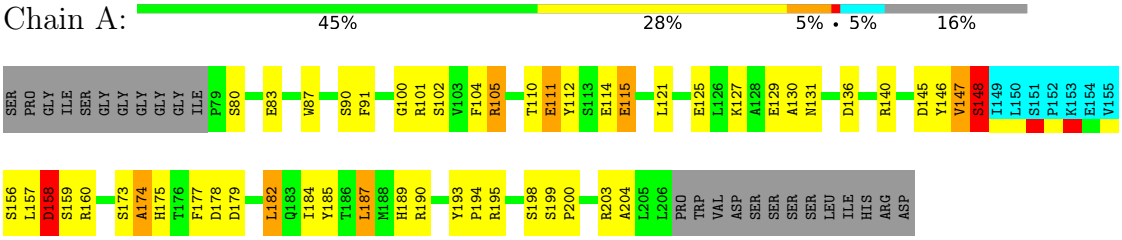
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)

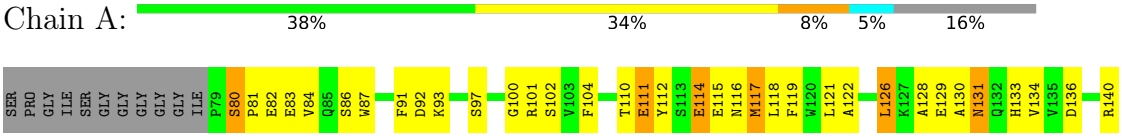
Chain A:

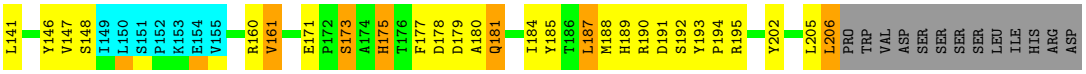


4.2.13 Score per residue for model 13

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)

Chain A:

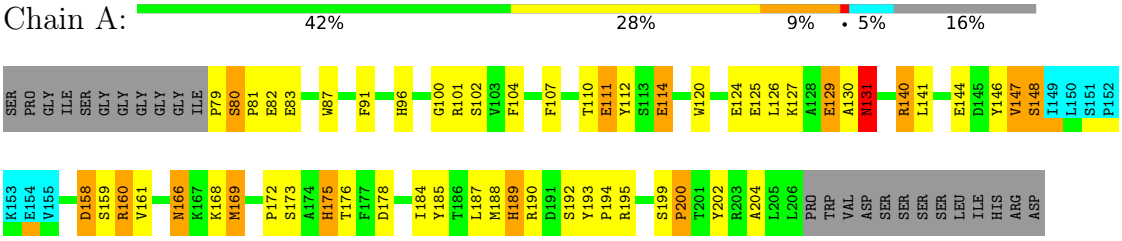




4.2.14 Score per residue for model 14

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)

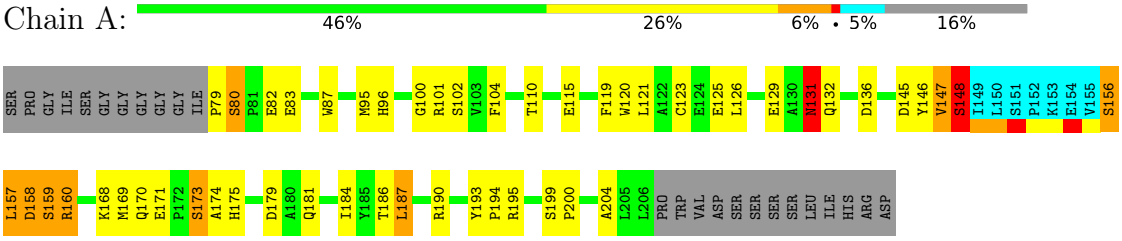
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)

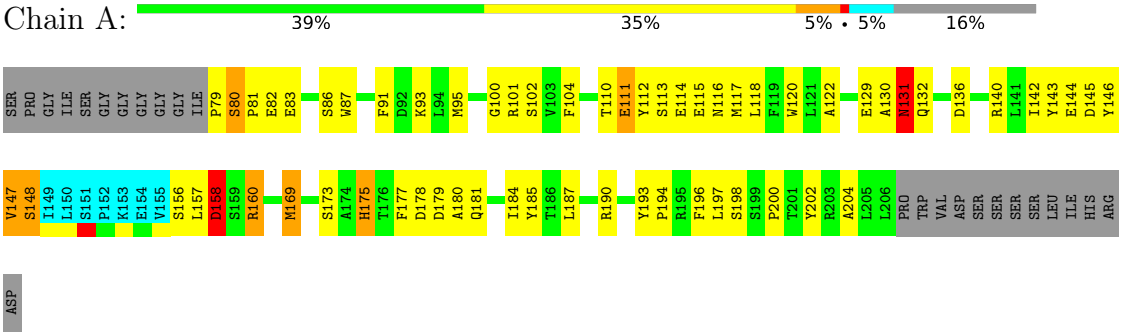
Chain A:



4.2.16 Score per residue for model 16

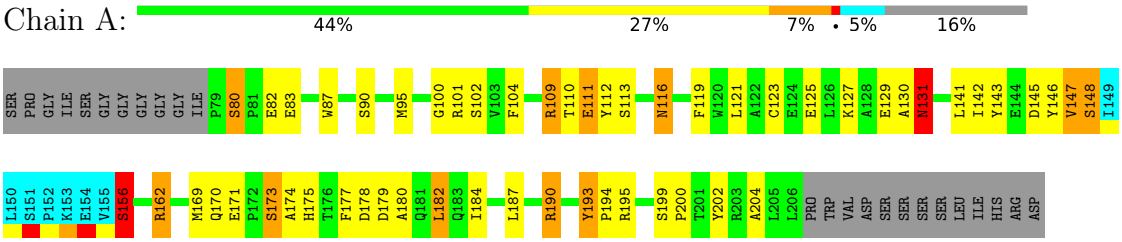
• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)

Chain A:



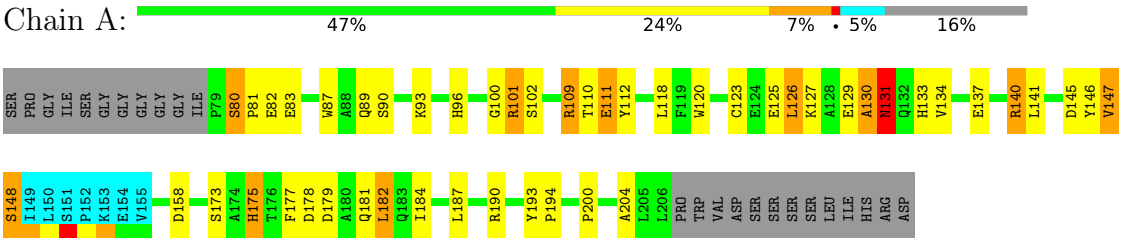
4.2.17 Score per residue for model 17

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



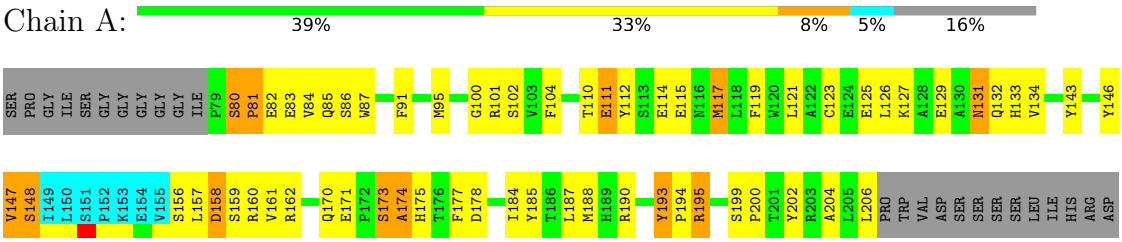
4.2.18 Score per residue for model 18

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



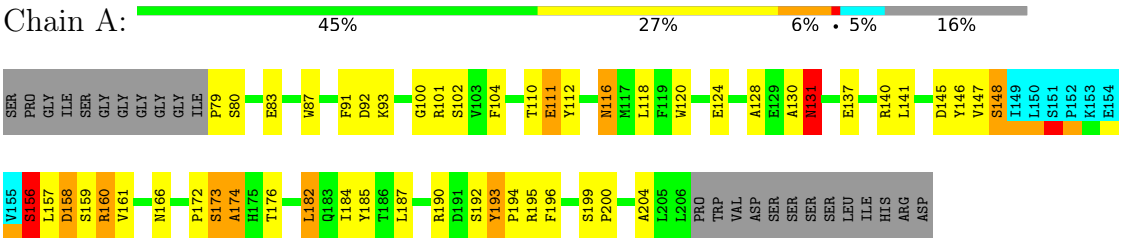
4.2.19 Score per residue for model 19

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



4.2.20 Score per residue for model 20

• Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY, SIMULATED ANNEALING*.

Of the 167 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	3.1
NMRPipe	structure solution	
PIPP	structure solution	
X-PLOR	structure solution	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	998	955	955	50±7
All	All	19960	19100	19100	998

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ASN:HD22	1:A:131:ASN:H	0.66	1.32	11	3
1:A:182:LEU:HD23	1:A:182:LEU:C	0.63	2.14	2	1
1:A:83:GLU:O	1:A:87:TRP:CG	0.63	2.52	10	20
1:A:131:ASN:ND2	1:A:131:ASN:H	0.62	1.92	15	12
1:A:189:HIS:NE2	1:A:193:TYR:CZ	0.62	2.67	4	2
1:A:131:ASN:HD22	1:A:131:ASN:N	0.61	1.93	11	2
1:A:120:TRP:CD1	1:A:181:GLN:NE2	0.61	2.68	4	1
1:A:189:HIS:NE2	1:A:190:ARG:NH2	0.61	2.48	13	1
1:A:173:SER:O	1:A:175:HIS:N	0.59	2.35	6	9
1:A:95:MET:SD	1:A:185:TYR:CZ	0.59	2.95	7	1
1:A:123:CYS:SG	1:A:181:GLN:NE2	0.58	2.76	18	1
1:A:129:GLU:O	1:A:130:ALA:HB3	0.58	1.98	17	3
1:A:111:GLU:O	1:A:112:TYR:CG	0.58	2.56	12	5
1:A:131:ASN:H	1:A:131:ASN:HD22	0.58	1.41	13	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:GLU:O	1:A:131:ASN:ND2	0.57	2.38	3	7
1:A:100:GLY:O	1:A:102:SER:N	0.57	2.37	20	18
1:A:91:PHE:CE2	1:A:185:TYR:CZ	0.57	2.93	8	1
1:A:133:HIS:CD2	1:A:134:VAL:N	0.57	2.73	19	2
1:A:189:HIS:CE1	1:A:190:ARG:HH21	0.57	2.17	13	1
1:A:189:HIS:CD2	1:A:193:TYR:CE1	0.56	2.93	6	1
1:A:131:ASN:ND2	1:A:131:ASN:N	0.56	2.53	13	9
1:A:146:TYR:O	1:A:148:SER:N	0.56	2.39	17	9
1:A:174:ALA:O	1:A:175:HIS:CG	0.56	2.59	10	2
1:A:129:GLU:O	1:A:131:ASN:N	0.56	2.39	6	8
1:A:200:PRO:O	1:A:204:ALA:HB2	0.55	2.01	4	18
1:A:140:ARG:O	1:A:144:GLU:N	0.55	2.39	2	5
1:A:195:ARG:O	1:A:199:SER:N	0.55	2.40	20	14
1:A:193:TYR:N	1:A:194:PRO:CD	0.55	2.70	1	18
1:A:95:MET:SD	1:A:120:TRP:CH2	0.54	3.00	16	1
1:A:95:MET:SD	1:A:120:TRP:CZ3	0.54	3.01	16	1
1:A:114:GLU:CD	1:A:114:GLU:H	0.54	2.05	14	1
1:A:174:ALA:O	1:A:176:THR:N	0.54	2.41	10	3
1:A:114:GLU:OE1	1:A:115:GLU:N	0.54	2.41	7	2
1:A:110:THR:O	1:A:112:TYR:N	0.54	2.41	10	14
1:A:114:GLU:N	1:A:114:GLU:OE2	0.54	2.40	7	1
1:A:89:GLN:NE2	1:A:93:LYS:NZ	0.54	2.56	18	1
1:A:159:SER:OG	1:A:160:ARG:N	0.53	2.41	4	5
1:A:128:ALA:O	1:A:130:ALA:N	0.53	2.41	10	3
1:A:110:THR:OG1	1:A:111:GLU:N	0.53	2.41	13	17
1:A:143:TYR:CZ	1:A:147:VAL:HG11	0.53	2.39	3	1
1:A:81:PRO:O	1:A:85:GLN:NE2	0.53	2.41	19	1
1:A:125:GLU:O	1:A:127:LYS:N	0.53	2.41	18	4
1:A:175:HIS:NE2	1:A:178:ASP:OD2	0.53	2.42	14	1
1:A:114:GLU:CD	1:A:115:GLU:N	0.53	2.62	7	1
1:A:121:LEU:O	1:A:125:GLU:N	0.53	2.42	19	8
1:A:98:PRO:O	1:A:101:ARG:NH1	0.53	2.42	6	1
1:A:175:HIS:H	1:A:175:HIS:CD2	0.53	2.22	7	1
1:A:165:ILE:HD12	1:A:165:ILE:N	0.53	2.18	10	1
1:A:116:ASN:N	1:A:116:ASN:OD1	0.53	2.41	20	1
1:A:200:PRO:O	1:A:204:ALA:N	0.53	2.42	2	9
1:A:145:ASP:OD2	1:A:146:TYR:CZ	0.53	2.62	8	6
1:A:197:LEU:O	1:A:203:ARG:NH2	0.53	2.41	3	1
1:A:79:PRO:N	1:A:83:GLU:OE1	0.53	2.42	15	2
1:A:179:ASP:OD1	1:A:180:ALA:N	0.53	2.42	7	6
1:A:184:ILE:O	1:A:187:LEU:N	0.52	2.42	18	12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:ASP:OD1	1:A:140:ARG:NH2	0.52	2.42	3	3
1:A:107:PHE:CE2	1:A:111:GLU:OE2	0.52	2.62	11	1
1:A:145:ASP:OD1	1:A:146:TYR:CE1	0.52	2.62	12	2
1:A:181:GLN:O	1:A:181:GLN:NE2	0.52	2.43	10	1
1:A:145:ASP:OD1	1:A:146:TYR:CZ	0.52	2.62	12	1
1:A:120:TRP:CZ3	1:A:124:GLU:OE1	0.52	2.62	20	2
1:A:143:TYR:OH	1:A:162:ARG:NH2	0.52	2.42	17	1
1:A:162:ARG:HH11	1:A:162:ARG:CG	0.52	2.18	17	1
1:A:92:ASP:OD1	1:A:93:LYS:N	0.52	2.42	20	5
1:A:145:ASP:O	1:A:146:TYR:CD1	0.52	2.62	3	3
1:A:166:ASN:HD22	1:A:166:ASN:N	0.52	2.02	14	2
1:A:124:GLU:OE1	1:A:127:LYS:NZ	0.52	2.42	8	1
1:A:129:GLU:N	1:A:129:GLU:OE1	0.52	2.41	14	1
1:A:145:ASP:OD2	1:A:146:TYR:CE2	0.52	2.62	16	6
1:A:105:ARG:NH1	1:A:105:ARG:CG	0.52	2.73	12	3
1:A:129:GLU:OE2	1:A:130:ALA:N	0.52	2.42	6	1
1:A:114:GLU:O	1:A:117:MET:N	0.52	2.43	6	5
1:A:82:GLU:N	1:A:82:GLU:OE1	0.52	2.42	2	1
1:A:198:SER:O	1:A:203:ARG:NH1	0.52	2.42	12	2
1:A:165:ILE:N	1:A:165:ILE:CD1	0.52	2.72	10	1
1:A:140:ARG:NH1	1:A:140:ARG:CG	0.52	2.72	1	7
1:A:175:HIS:CD2	1:A:178:ASP:OD1	0.52	2.62	3	1
1:A:162:ARG:NH1	1:A:162:ARG:CG	0.52	2.72	7	1
1:A:175:HIS:O	1:A:175:HIS:CD2	0.52	2.62	15	1
1:A:158:ASP:OD2	1:A:162:ARG:NH2	0.52	2.43	19	1
1:A:136:ASP:OD2	1:A:140:ARG:NH2	0.52	2.43	13	3
1:A:111:GLU:OE1	1:A:195:ARG:NH2	0.52	2.42	11	1
1:A:160:ARG:CG	1:A:160:ARG:NH1	0.52	2.72	16	2
1:A:114:GLU:OE2	1:A:115:GLU:N	0.52	2.42	13	1
1:A:120:TRP:CH2	1:A:124:GLU:OE1	0.52	2.62	14	1
1:A:160:ARG:CG	1:A:160:ARG:HH11	0.52	2.17	16	2
1:A:86:SER:OG	1:A:93:LYS:NZ	0.52	2.42	16	1
1:A:191:ASP:O	1:A:195:ARG:NH1	0.52	2.42	11	1
1:A:109:ARG:NH1	1:A:109:ARG:CG	0.52	2.73	18	3
1:A:195:ARG:NH1	1:A:195:ARG:CG	0.52	2.72	7	3
1:A:116:ASN:HD21	1:A:184:ILE:CG2	0.52	2.18	17	1
1:A:110:THR:O	1:A:112:TYR:CD2	0.52	2.63	13	1
1:A:137:GLU:OE2	1:A:140:ARG:NH2	0.52	2.42	20	1
1:A:129:GLU:CD	1:A:130:ALA:N	0.51	2.63	6	1
1:A:157:LEU:HD22	1:A:157:LEU:N	0.51	2.20	11	1
1:A:137:GLU:H	1:A:137:GLU:CD	0.51	2.09	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:PHE:CD1	1:A:185:TYR:OH	0.51	2.61	19	9
1:A:131:ASN:N	1:A:131:ASN:ND2	0.51	2.57	11	2
1:A:162:ARG:CG	1:A:162:ARG:HH11	0.51	2.18	7	1
1:A:140:ARG:CG	1:A:140:ARG:HH11	0.51	2.18	1	8
1:A:83:GLU:O	1:A:87:TRP:CD1	0.51	2.64	7	3
1:A:162:ARG:CG	1:A:162:ARG:NH1	0.51	2.72	17	1
1:A:115:GLU:H	1:A:115:GLU:CD	0.51	2.09	15	3
1:A:120:TRP:CZ2	1:A:124:GLU:OE2	0.51	2.63	14	1
1:A:157:LEU:O	1:A:162:ARG:NH2	0.51	2.43	4	1
1:A:203:ARG:NH1	1:A:203:ARG:CG	0.51	2.73	6	1
1:A:102:SER:OG	1:A:103:VAL:N	0.51	2.43	10	2
1:A:195:ARG:CG	1:A:195:ARG:HH11	0.51	2.18	4	4
1:A:110:THR:C	1:A:112:TYR:H	0.51	2.09	10	17
1:A:80:SER:N	1:A:83:GLU:OE1	0.51	2.43	9	2
1:A:119:PHE:O	1:A:181:GLN:NE2	0.51	2.44	13	1
1:A:80:SER:O	1:A:82:GLU:N	0.50	2.44	13	14
1:A:115:GLU:CD	1:A:115:GLU:N	0.50	2.65	12	4
1:A:189:HIS:O	1:A:189:HIS:ND1	0.50	2.41	14	1
1:A:175:HIS:CE1	1:A:178:ASP:CB	0.50	2.94	18	1
1:A:190:ARG:O	1:A:190:ARG:NE	0.50	2.42	6	1
1:A:169:MET:SD	1:A:169:MET:O	0.50	2.69	8	7
1:A:105:ARG:NH2	1:A:114:GLU:OE2	0.50	2.45	12	2
1:A:85:GLN:N	1:A:85:GLN:OE1	0.50	2.44	19	1
1:A:101:ARG:NH1	1:A:101:ARG:CG	0.50	2.73	6	1
1:A:160:ARG:NH1	1:A:160:ARG:CG	0.50	2.72	15	2
1:A:190:ARG:NH1	1:A:190:ARG:CG	0.50	2.72	17	2
1:A:101:ARG:CG	1:A:101:ARG:HH11	0.50	2.19	6	1
1:A:115:GLU:CG	1:A:116:ASN:N	0.50	2.75	8	1
1:A:96:HIS:O	1:A:96:HIS:ND1	0.50	2.44	15	2
1:A:190:ARG:O	1:A:194:PRO:CG	0.49	2.60	7	13
1:A:179:ASP:OD1	1:A:179:ASP:N	0.49	2.45	7	2
1:A:145:ASP:OD1	1:A:146:TYR:CD2	0.49	2.65	16	1
1:A:173:SER:OG	1:A:175:HIS:NE2	0.49	2.44	1	1
1:A:195:ARG:CG	1:A:195:ARG:NH1	0.49	2.72	4	1
1:A:177:PHE:O	1:A:181:GLN:N	0.49	2.37	3	1
1:A:109:ARG:CG	1:A:109:ARG:HH11	0.49	2.21	18	2
1:A:92:ASP:O	1:A:96:HIS:N	0.49	2.42	11	1
1:A:196:PHE:O	1:A:198:SER:N	0.49	2.46	16	1
1:A:168:LYS:O	1:A:170:GLN:N	0.49	2.46	15	3
1:A:129:GLU:C	1:A:131:ASN:ND2	0.49	2.66	2	4
1:A:157:LEU:O	1:A:158:ASP:CB	0.49	2.61	1	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:LYS:CB	1:A:167:LYS:NZ	0.49	2.76	8	2
1:A:175:HIS:CD2	1:A:178:ASP:OD2	0.49	2.66	14	1
1:A:92:ASP:CG	1:A:93:LYS:N	0.49	2.67	2	3
1:A:189:HIS:ND1	1:A:189:HIS:O	0.49	2.45	8	2
1:A:173:SER:OG	1:A:175:HIS:CE1	0.49	2.65	16	1
1:A:109:ARG:HH11	1:A:109:ARG:CG	0.49	2.19	3	2
1:A:147:VAL:O	1:A:148:SER:O	0.49	2.31	19	17
1:A:105:ARG:CG	1:A:105:ARG:HH11	0.49	2.21	7	3
1:A:190:ARG:CG	1:A:190:ARG:HH11	0.48	2.20	17	1
1:A:109:ARG:CG	1:A:109:ARG:NH1	0.48	2.72	3	2
1:A:117:MET:C	1:A:117:MET:SD	0.48	2.91	19	2
1:A:119:PHE:O	1:A:123:CYS:SG	0.48	2.71	17	4
1:A:129:GLU:C	1:A:131:ASN:HD22	0.48	2.12	6	3
1:A:111:GLU:C	1:A:112:TYR:CD2	0.48	2.87	6	5
1:A:129:GLU:CD	1:A:130:ALA:H	0.48	2.12	6	1
1:A:129:GLU:CA	1:A:131:ASN:ND2	0.48	2.77	2	3
1:A:162:ARG:O	1:A:166:ASN:ND2	0.48	2.47	3	1
1:A:114:GLU:CD	1:A:114:GLU:N	0.48	2.67	13	2
1:A:120:TRP:O	1:A:123:CYS:SG	0.48	2.69	18	1
1:A:114:GLU:O	1:A:116:ASN:N	0.48	2.46	10	2
1:A:160:ARG:CG	1:A:161:VAL:N	0.48	2.76	13	1
1:A:82:GLU:O	1:A:86:SER:N	0.48	2.41	13	2
1:A:117:MET:O	1:A:121:LEU:N	0.48	2.39	4	1
1:A:181:GLN:CG	1:A:182:LEU:N	0.48	2.77	8	1
1:A:114:GLU:OE1	1:A:114:GLU:N	0.48	2.41	14	1
1:A:83:GLU:O	1:A:87:TRP:CD2	0.48	2.66	19	5
1:A:116:ASN:OD1	1:A:117:MET:N	0.48	2.46	11	2
1:A:100:GLY:C	1:A:102:SER:N	0.47	2.68	6	19
1:A:159:SER:O	1:A:161:VAL:N	0.47	2.48	20	7
1:A:129:GLU:OE1	1:A:129:GLU:CA	0.47	2.62	14	1
1:A:140:ARG:CG	1:A:140:ARG:NH1	0.47	2.72	14	1
1:A:146:TYR:O	1:A:147:VAL:C	0.47	2.53	18	17
1:A:129:GLU:O	1:A:130:ALA:CB	0.47	2.62	17	3
1:A:79:PRO:N	1:A:83:GLU:CD	0.47	2.68	6	1
1:A:190:ARG:O	1:A:194:PRO:CD	0.47	2.62	8	1
1:A:111:GLU:O	1:A:113:SER:N	0.47	2.46	10	2
1:A:203:ARG:CG	1:A:203:ARG:HH11	0.47	2.22	6	1
1:A:133:HIS:CG	1:A:134:VAL:N	0.47	2.83	19	2
1:A:82:GLU:N	1:A:82:GLU:CD	0.47	2.68	2	1
1:A:96:HIS:ND1	1:A:96:HIS:N	0.47	2.62	9	2
1:A:79:PRO:CD	1:A:83:GLU:OE2	0.47	2.62	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:HIS:ND1	1:A:175:HIS:C	0.47	2.66	11	1
1:A:129:GLU:C	1:A:131:ASN:N	0.47	2.67	2	9
1:A:189:HIS:ND1	1:A:193:TYR:CE1	0.47	2.83	8	1
1:A:174:ALA:O	1:A:175:HIS:ND1	0.47	2.48	12	1
1:A:92:ASP:OD1	1:A:92:ASP:N	0.47	2.48	3	3
1:A:157:LEU:N	1:A:157:LEU:CD2	0.47	2.78	11	1
1:A:157:LEU:HD13	1:A:158:ASP:N	0.47	2.25	15	1
1:A:110:THR:O	1:A:112:TYR:CD1	0.47	2.68	17	2
1:A:168:LYS:NZ	1:A:176:THR:OG1	0.47	2.42	14	1
1:A:137:GLU:CD	1:A:140:ARG:NH2	0.47	2.68	20	1
1:A:80:SER:C	1:A:82:GLU:H	0.46	2.13	1	13
1:A:143:TYR:CD1	1:A:143:TYR:O	0.46	2.67	6	2
1:A:174:ALA:C	1:A:176:THR:N	0.46	2.68	10	3
1:A:177:PHE:O	1:A:178:ASP:C	0.46	2.53	7	12
1:A:96:HIS:CG	1:A:96:HIS:O	0.46	2.69	5	1
1:A:111:GLU:C	1:A:112:TYR:CG	0.46	2.88	12	8
1:A:123:CYS:SG	1:A:124:GLU:N	0.46	2.88	8	1
1:A:125:GLU:C	1:A:127:LYS:H	0.46	2.13	14	2
1:A:129:GLU:C	1:A:131:ASN:H	0.46	2.14	19	8
1:A:107:PHE:CZ	1:A:111:GLU:OE1	0.46	2.68	7	1
1:A:171:GLU:N	1:A:171:GLU:OE2	0.46	2.49	13	1
1:A:196:PHE:C	1:A:198:SER:N	0.46	2.68	16	1
1:A:119:PHE:CD1	1:A:119:PHE:C	0.46	2.88	10	1
1:A:80:SER:C	1:A:82:GLU:N	0.46	2.69	13	15
1:A:173:SER:OG	1:A:174:ALA:N	0.46	2.48	7	2
1:A:173:SER:C	1:A:175:HIS:N	0.46	2.69	15	2
1:A:189:HIS:CE1	1:A:190:ARG:NH2	0.46	2.83	12	2
1:A:110:THR:C	1:A:112:TYR:N	0.46	2.69	5	13
1:A:175:HIS:N	1:A:175:HIS:ND1	0.46	2.64	2	2
1:A:125:GLU:C	1:A:127:LYS:N	0.46	2.69	14	4
1:A:83:GLU:N	1:A:83:GLU:CD	0.46	2.69	9	6
1:A:173:SER:OG	1:A:175:HIS:CD2	0.46	2.68	1	1
1:A:147:VAL:O	1:A:148:SER:C	0.46	2.53	6	3
1:A:202:TYR:C	1:A:202:TYR:CD1	0.46	2.88	9	4
1:A:105:ARG:HH21	1:A:118:LEU:CD2	0.46	2.23	7	1
1:A:116:ASN:OD1	1:A:184:ILE:CG2	0.46	2.64	13	2
1:A:168:LYS:NZ	1:A:176:THR:CB	0.46	2.79	14	1
1:A:143:TYR:CE1	1:A:147:VAL:HG11	0.46	2.46	19	1
1:A:173:SER:O	1:A:174:ALA:O	0.46	2.34	20	3
1:A:115:GLU:CD	1:A:115:GLU:H	0.46	2.14	5	2
1:A:168:LYS:O	1:A:171:GLU:N	0.45	2.43	4	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:184:ILE:O	1:A:188:MET:SD	0.45	2.74	5	1
1:A:85:GLN:N	1:A:85:GLN:CD	0.45	2.69	19	1
1:A:182:LEU:C	1:A:182:LEU:HD13	0.45	2.32	11	1
1:A:156:SER:OG	1:A:187:LEU:CD1	0.45	2.64	15	1
1:A:193:TYR:N	1:A:194:PRO:HD2	0.45	2.27	17	19
1:A:115:GLU:N	1:A:115:GLU:OE2	0.45	2.49	5	2
1:A:173:SER:C	1:A:175:HIS:H	0.45	2.15	12	1
1:A:141:LEU:N	1:A:141:LEU:CD2	0.45	2.80	4	4
1:A:157:LEU:O	1:A:158:ASP:O	0.45	2.35	8	1
1:A:177:PHE:O	1:A:179:ASP:N	0.45	2.50	1	1
1:A:141:LEU:O	1:A:141:LEU:HD23	0.45	2.11	20	2
1:A:142:ILE:O	1:A:145:ASP:OD1	0.44	2.35	16	3
1:A:188:MET:O	1:A:192:SER:N	0.44	2.41	2	1
1:A:82:GLU:O	1:A:86:SER:OG	0.44	2.36	19	3
1:A:169:MET:C	1:A:169:MET:SD	0.44	2.96	3	1
1:A:141:LEU:HD12	1:A:141:LEU:N	0.44	2.27	17	2
1:A:96:HIS:N	1:A:96:HIS:ND1	0.44	2.65	11	1
1:A:184:ILE:O	1:A:186:THR:N	0.44	2.50	11	1
1:A:175:HIS:CD2	1:A:175:HIS:N	0.44	2.84	7	1
1:A:174:ALA:C	1:A:176:THR:H	0.44	2.16	20	2
1:A:86:SER:OG	1:A:93:LYS:CD	0.44	2.65	16	2
1:A:141:LEU:N	1:A:141:LEU:HD22	0.44	2.27	4	2
1:A:123:CYS:SG	1:A:181:GLN:CD	0.44	2.96	5	1
1:A:129:GLU:OE2	1:A:131:ASN:ND2	0.44	2.50	11	1
1:A:160:ARG:HH11	1:A:160:ARG:CB	0.44	2.26	11	1
1:A:120:TRP:NE1	1:A:181:GLN:NE2	0.44	2.65	15	1
1:A:200:PRO:O	1:A:204:ALA:CB	0.44	2.66	1	4
1:A:192:SER:O	1:A:196:PHE:CB	0.44	2.66	20	5
1:A:114:GLU:CD	1:A:115:GLU:H	0.44	2.16	7	1
1:A:171:GLU:N	1:A:171:GLU:CD	0.44	2.71	13	1
1:A:177:PHE:O	1:A:180:ALA:N	0.44	2.50	1	2
1:A:173:SER:O	1:A:174:ALA:HB2	0.44	2.13	9	1
1:A:98:PRO:N	1:A:101:ARG:HH21	0.44	2.10	2	1
1:A:170:GLN:O	1:A:171:GLU:C	0.44	2.55	2	1
1:A:173:SER:O	1:A:174:ALA:HB3	0.44	2.13	5	3
1:A:160:ARG:HH11	1:A:160:ARG:CG	0.44	2.24	11	1
1:A:157:LEU:O	1:A:158:ASP:OD1	0.44	2.35	15	2
1:A:175:HIS:O	1:A:178:ASP:OD2	0.43	2.36	3	2
1:A:158:ASP:O	1:A:159:SER:CB	0.43	2.64	4	1
1:A:158:ASP:O	1:A:159:SER:OG	0.43	2.36	20	2
1:A:146:TYR:O	1:A:148:SER:O	0.43	2.37	13	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:GLU:CG	1:A:130:ALA:H	0.43	2.25	6	1
1:A:95:MET:SD	1:A:185:TYR:OH	0.43	2.77	7	1
1:A:145:ASP:OD1	1:A:145:ASP:O	0.43	2.36	12	1
1:A:175:HIS:ND1	1:A:175:HIS:N	0.43	2.67	19	1
1:A:159:SER:C	1:A:161:VAL:N	0.43	2.69	20	7
1:A:130:ALA:O	1:A:131:ASN:O	0.43	2.36	18	6
1:A:145:ASP:O	1:A:145:ASP:OD1	0.43	2.37	4	6
1:A:158:ASP:O	1:A:159:SER:O	0.43	2.37	5	2
1:A:118:LEU:O	1:A:122:ALA:N	0.43	2.41	16	1
1:A:129:GLU:OE1	1:A:134:VAL:O	0.43	2.37	18	1
1:A:166:ASN:OD1	1:A:166:ASN:O	0.43	2.36	20	1
1:A:136:ASP:CG	1:A:140:ARG:NH2	0.43	2.72	3	1
1:A:202:TYR:CD1	1:A:202:TYR:C	0.43	2.91	19	5
1:A:196:PHE:C	1:A:198:SER:H	0.43	2.16	16	1
1:A:175:HIS:O	1:A:178:ASP:OD1	0.43	2.37	18	1
1:A:175:HIS:NE2	1:A:178:ASP:OD1	0.43	2.51	3	1
1:A:184:ILE:C	1:A:186:THR:N	0.43	2.72	9	3
1:A:135:VAL:O	1:A:139:ALA:CB	0.43	2.67	9	1
1:A:168:LYS:HZ2	1:A:176:THR:CB	0.43	2.27	14	1
1:A:115:GLU:OE2	1:A:116:ASN:N	0.43	2.52	2	1
1:A:187:LEU:O	1:A:187:LEU:HD23	0.43	2.14	6	2
1:A:114:GLU:N	1:A:114:GLU:CD	0.43	2.72	7	1
1:A:124:GLU:OE2	1:A:181:GLN:OE1	0.43	2.37	8	1
1:A:158:ASP:O	1:A:158:ASP:OD1	0.43	2.37	11	1
1:A:113:SER:O	1:A:113:SER:OG	0.43	2.37	17	1
1:A:144:GLU:O	1:A:148:SER:OG	0.42	2.36	11	2
1:A:108:LEU:O	1:A:109:ARG:C	0.42	2.57	9	2
1:A:141:LEU:N	1:A:141:LEU:CD1	0.42	2.81	17	2
1:A:191:ASP:OD1	1:A:195:ARG:NH2	0.42	2.52	13	1
1:A:132:GLN:O	1:A:132:GLN:NE2	0.42	2.52	4	1
1:A:98:PRO:O	1:A:102:SER:OG	0.42	2.38	6	1
1:A:125:GLU:O	1:A:129:GLU:OE1	0.42	2.37	7	1
1:A:182:LEU:C	1:A:182:LEU:CD1	0.42	2.88	11	5
1:A:170:GLN:N	1:A:170:GLN:CD	0.42	2.73	9	1
1:A:80:SER:O	1:A:83:GLU:OE1	0.42	2.38	10	1
1:A:107:PHE:CE2	1:A:111:GLU:OE1	0.42	2.72	14	1
1:A:168:LYS:CB	1:A:176:THR:OG1	0.42	2.67	14	1
1:A:126:LEU:HD12	1:A:129:GLU:OE2	0.42	2.15	18	1
1:A:105:ARG:NH2	1:A:118:LEU:CD2	0.42	2.83	7	1
1:A:82:GLU:O	1:A:86:SER:CB	0.42	2.67	13	2
1:A:188:MET:O	1:A:192:SER:OG	0.42	2.35	14	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:THR:CG2	1:A:190:ARG:NH2	0.42	2.82	15	1
1:A:173:SER:O	1:A:173:SER:OG	0.42	2.31	20	1
1:A:109:ARG:C	1:A:109:ARG:CD	0.42	2.88	6	1
1:A:114:GLU:O	1:A:115:GLU:C	0.42	2.58	19	6
1:A:125:GLU:O	1:A:128:ALA:N	0.42	2.41	10	1
1:A:114:GLU:OE2	1:A:114:GLU:O	0.42	2.37	11	1
1:A:178:ASP:CG	1:A:179:ASP:H	0.42	2.18	18	1
1:A:93:LYS:O	1:A:97:SER:OG	0.42	2.36	13	1
1:A:126:LEU:HD23	1:A:126:LEU:O	0.42	2.14	13	1
1:A:178:ASP:O	1:A:182:LEU:N	0.42	2.49	17	1
1:A:129:GLU:CG	1:A:130:ALA:N	0.42	2.83	6	1
1:A:195:ARG:O	1:A:199:SER:OG	0.42	2.36	14	2
1:A:157:LEU:O	1:A:158:ASP:CG	0.42	2.58	16	3
1:A:184:ILE:HG22	1:A:188:MET:SD	0.42	2.55	19	1
1:A:106:ALA:O	1:A:107:PHE:C	0.41	2.59	6	1
1:A:105:ARG:NH2	1:A:118:LEU:HD23	0.41	2.30	7	1
1:A:124:GLU:OE2	1:A:124:GLU:O	0.41	2.38	9	1
1:A:133:HIS:CD2	1:A:133:HIS:H	0.41	2.32	13	1
1:A:170:GLN:O	1:A:171:GLU:OE2	0.41	2.38	19	2
1:A:178:ASP:CG	1:A:179:ASP:N	0.41	2.73	18	1
1:A:131:ASN:O	1:A:132:GLN:OE1	0.41	2.37	19	1
1:A:206:LEU:C	1:A:206:LEU:HD23	0.41	2.35	6	1
1:A:114:GLU:C	1:A:116:ASN:N	0.41	2.72	10	1
1:A:184:ILE:CG2	1:A:185:TYR:N	0.41	2.84	4	1
1:A:206:LEU:C	1:A:206:LEU:CD1	0.41	2.89	7	2
1:A:127:LYS:NZ	1:A:127:LYS:CB	0.41	2.83	12	1
1:A:111:GLU:O	1:A:112:TYR:C	0.41	2.59	7	1
1:A:133:HIS:CD2	1:A:134:VAL:H	0.41	2.34	19	1
1:A:157:LEU:HD11	1:A:183:GLN:NE2	0.41	2.31	9	1
1:A:128:ALA:O	1:A:129:GLU:OE2	0.41	2.38	2	1
1:A:143:TYR:CZ	1:A:147:VAL:CG1	0.41	3.03	3	1
1:A:105:ARG:NH1	1:A:114:GLU:OE1	0.41	2.54	6	1
1:A:196:PHE:CD1	1:A:196:PHE:C	0.41	2.94	10	1
1:A:120:TRP:HE1	1:A:181:GLN:HE21	0.41	1.58	16	1
1:A:158:ASP:N	1:A:158:ASP:OD1	0.41	2.53	18	1
1:A:146:TYR:O	1:A:147:VAL:CG2	0.41	2.68	19	1
1:A:138:LYS:C	1:A:140:ARG:N	0.41	2.74	6	1
1:A:175:HIS:O	1:A:175:HIS:CG	0.41	2.73	15	1
1:A:140:ARG:O	1:A:141:LEU:C	0.40	2.60	7	4
1:A:156:SER:O	1:A:157:LEU:C	0.40	2.59	10	1
1:A:199:SER:C	1:A:203:ARG:HH12	0.40	2.19	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:GLU:CD	1:A:137:GLU:N	0.40	2.73	18	1
1:A:116:ASN:OD1	1:A:116:ASN:N	0.40	2.53	5	2
1:A:121:LEU:O	1:A:122:ALA:C	0.40	2.59	13	1
1:A:184:ILE:O	1:A:185:TYR:C	0.40	2.60	11	1
1:A:159:SER:O	1:A:160:ARG:C	0.40	2.60	20	1
1:A:159:SER:O	1:A:162:ARG:N	0.40	2.52	2	1
1:A:95:MET:SD	1:A:185:TYR:CE1	0.40	3.14	7	1
1:A:143:TYR:CD1	1:A:143:TYR:C	0.40	2.94	11	1
1:A:146:TYR:C	1:A:148:SER:N	0.40	2.74	11	2
1:A:189:HIS:CD2	1:A:190:ARG:NH2	0.40	2.89	13	1
1:A:194:PRO:C	1:A:195:ARG:HE	0.40	2.18	19	1
1:A:100:GLY:O	1:A:101:ARG:C	0.40	2.60	18	1
1:A:133:HIS:O	1:A:137:GLU:OE1	0.40	2.39	18	1
1:A:137:GLU:CD	1:A:140:ARG:HH21	0.40	2.18	20	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/152 (78%)	93±2 (78±2%)	16±2 (14±2%)	9±2 (8±2%)	2	14
All	All	2380/3040 (78%)	1863 (78%)	330 (14%)	187 (8%)	2	14

All 23 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	148	SER	18
1	A	111	GLU	17
1	A	131	ASN	17
1	A	101	ARG	17
1	A	147	VAL	16
1	A	158	ASP	15
1	A	173	SER	14
1	A	156	SER	11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	81	PRO	9
1	A	132	GLN	9
1	A	174	ALA	9
1	A	159	SER	7
1	A	130	ALA	7
1	A	175	HIS	6
1	A	172	PRO	5
1	A	169	MET	2
1	A	126	LEU	2
1	A	178	ASP	1
1	A	112	TYR	1
1	A	115	GLU	1
1	A	157	LEU	1
1	A	129	GLU	1
1	A	197	LEU	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/134 (81%)	99±2 (90±2%)	10±2 (10±2%)	12	58
All	All	2180/2680 (81%)	1972 (90%)	208 (10%)	12	58

All 53 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	80	SER	20
1	A	104	PHE	17
1	A	131	ASN	14
1	A	160	ARG	9
1	A	187	LEU	9
1	A	158	ASP	8
1	A	95	MET	8
1	A	169	MET	8
1	A	109	ARG	6
1	A	118	LEU	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	193	TYR	6
1	A	90	SER	5
1	A	79	PRO	5
1	A	182	LEU	5
1	A	136	ASP	4
1	A	126	LEU	4
1	A	96	HIS	4
1	A	115	GLU	3
1	A	179	ASP	3
1	A	195	ARG	3
1	A	185	TYR	3
1	A	105	ARG	3
1	A	114	GLU	3
1	A	175	HIS	3
1	A	206	LEU	3
1	A	117	MET	3
1	A	148	SER	3
1	A	156	SER	3
1	A	110	THR	2
1	A	176	THR	2
1	A	132	GLN	2
1	A	138	LYS	2
1	A	203	ARG	2
1	A	129	GLU	2
1	A	184	ILE	2
1	A	162	ARG	2
1	A	205	LEU	2
1	A	84	VAL	2
1	A	140	ARG	2
1	A	116	ASN	2
1	A	82	GLU	1
1	A	167	LYS	1
1	A	171	GLU	1
1	A	121	LEU	1
1	A	101	ARG	1
1	A	97	SER	1
1	A	161	VAL	1
1	A	181	GLN	1
1	A	166	ASN	1
1	A	189	HIS	1
1	A	200	PRO	1
1	A	157	LEU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	190	ARG	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided